

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.90e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.12e-01

Confidence level: 5.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>phenyl heptopyranoside</div> <div>Measured: 2.79e-02</div> <div>Predicted: 1.26e-01</div>	<div>Image not found</div> <div>Dexpanthenol</div> <div>Measured: 4.87</div> <div>Predicted: 3.46</div>	<div>Image not found</div> <div>4-[Cyclopropyl(hydroxy)methylidene]-3,5-dioxocyclohexane-1-carboxylic acid</div> <div>Measured: 5.80e-03</div> <div>Predicted: 7.67e-03</div>
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